Chlorthal-dimethyl

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 345 °C

Global applicability domain: Inside

Local applicability domain index: 4.36e-01

Confidence level: 6.28e-01

Nearest Neighbors from the Training Set

Image not found
Chlorthal-dimethyl
Measured: 365
Predicted: 345

Image not found
Phosphine, ethyldiphenyl-
Measured: 293
Predicted: 310

Image not found
Di(2-methoxyethyl) phthalate
Measured: 340
Predicted: 332

Image not found
Benzeneacetic acid, (4-methoxyphenyl)methyl ester
Measured: 370
Predicted: 342

Image not found
4-Bromobenzophenone
Measured: 350
Predicted: 336